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Parallel ABS Projection Methods for Linear and Nonlinear Systems with Block Arrowhead Structure

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Abstract—We investigate the implementation of the block implicit LU ABS methods on linear and nonlinear algebraic systems with block arrowhead coefficient or Jacobian matrix. Connections with other methods specialized for such problems are investigated in detail. It is shown that the block implicit LU ABS method contains Method 2 of Schmidt and Hoyer [1], the basic corrected implicit method of Zhang *et al.* [2], and the capacitance matrix method of Bjørstad and Widlund [3], as special cases. Experimental results which indicate the usefulness of the method are also mentioned.

Keywords—Nonlinear systems, Structured sparsity, Capacitance matrix, LU ABS method.

1. INTRODUCTION

We investigate the numerical solution of the block bordered nonlinear systems of the form

$$\begin{aligned} f_i(x_i, x_{q+1}) &= 0, \qquad i = 1, \dots, q, \\ f_{q+1}(x_1, \dots, x_{q+1}) &= 0, \end{aligned} \tag{1}$$

where $x_i \in R^{n_i}$, $f_i \in R^{n_i}$ $(i = 1, \dots, q+1)$, and $\sum_{i=1}^{q+1} n_i = n$. Such systems of nonlinear equations occur in VLSI design and other application areas (see [1,2,4] and the references therein). Let $\mathbf{x} = [x_1^\top, \dots, x_q^\top, x_{q+1}^\top]^\top \in R^n$ and

$$F(\mathbf{x}) = \left[f_1^\top(x), \dots, f_q^\top(x), f_{q+1}^\top(x)\right]^\top \in R^n, \tag{2}$$

where the superscript $\top$ denotes the transpose. Then the Jacobian matrix of system (1) has the block bordered or arrowhead structure

$$J(\mathbf{x}) = \begin{bmatrix} A_1 & & & & B_1 \\ & A_2 & & & B_2 \\ & & \ddots & & \vdots \\ & & & A_q & B_q \\ C_1 & C_2 & \dots & C_q & D \end{bmatrix}, \tag{3}$$

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where

$$A_i = \frac{\partial f_i(\mathbf{x})}{\partial x_i} \in R^{n_i \times n_i} \qquad (i = 1, \dots, q), \qquad D = \frac{\partial f_{q+1}(\mathbf{x})}{\partial x_{q+1}} \in R^{n_{q+1} \times n_{q+1}}, \tag{4}$$

and

$$B_i = \frac{\partial f_i(\mathbf{x})}{\partial x_{q+1}} \in R^{n_i \times n_{q+1}}, \quad C_i = \frac{\partial f_{q+1}(\mathbf{x})}{\partial x_i} \in R^{n_{q+1} \times n_i}, \qquad (i = 1, \dots, q). \tag{5}$$

Linear systems with similar coefficient matrices arise in the domain decomposition method [3,5]. The special sparsity pattern of the Jacobian or the coefficient matrix (3) offers advantages for a specialized solver. Several authors investigated the efficient solution of such nonlinear systems for reasons of applications and algorithmic developments (see, e.g., [1,2,4,6–10]).

In this paper, we specialize the block implicit LU ABS algorithm to block bordered systems and compare it to the other existing methods. We show that Method 2 of Hoyer and Schmidt [1], which is equivalent with the basic corrected implicit method of Zhang *et al.* [2], is a special case of the block implicit LU ABS method. For block arrowhead linear systems, we demonstrate that the implicit LU ABS method also contains the capacitance matrix method of Bjørstad and Widlund [3]. The results indicate the usefulness of block ABS methods on systems with structured sparsity.

2. THE BASIC SOLUTION METHODS

The basic idea of the known methods is exploiting the implicit function theorem. The idea goes back to Brown [11] (see also [6,12]). Let

$$S(\mathbf{x}) = D(\mathbf{x}) - \sum_{i=1}^{q} C_i(\mathbf{x}) A_i^{-1}(\mathbf{x}) B_i(\mathbf{x}). \tag{6}$$

Hoyer and Schmidt suggested the following general algorithm to solve problems of the form (1).

Algorithm 1

Step 1. Solve $f_i(x_i, x_{q+1}) + A_i(\mathbf{x})(\tilde{x}_i - x_i) = 0$ for $\tilde{x}_i$ $(i = 1, \dots, q)$.
Step 2. Solve $f_{q+1}(\tilde{x}_1, \dots, \tilde{x}_q, x_{q+1}) + S(\mathbf{x})(x_{q+1}^+ - x_{q+1}) = 0$ for x_{q+1}^+.
Step 3. $x_i^+ = \Psi_i\left(\mathbf{x}, \tilde{x}_1, \dots, \tilde{x}_q, x_{q+1}^+\right)$ $(i = 1, \dots, q)$ (correction step).

The three corrections of Hoyer and Schmidt have the following forms:

$$x_i^+ = \tilde{x}_i, \qquad i = 1, \dots, q \text{ (Method 1)}, \tag{7}$$

$$x_i^+ = \tilde{x}_i - A_i(\mathbf{x})^{-1} B_i(\mathbf{x}) \left(x_{q+1}^+ - x_{q+1}\right), \qquad i = 1, \dots, q \text{ (Method 2)}, \tag{8}$$

$$f_i\left(\tilde{x}_i, x_{q+1}^+\right) + A_i(\mathbf{x})\left(x_i^+ - \tilde{x}_i\right) = 0, \qquad i = 1, \dots, q \text{ (Method 3)}. \tag{9}$$

Methods 1 and 2 are identical with the explicit and the basic corrected implicit methods of Zhang *et al.* [2], respectively. Hoyer and Schmidt [1] proved that the local convergence rate of Method 1 is 2-step Q-quadratic, while Methods 2 and 3 have local convergence of Q-order 2. Steps 1 and 3 of Algorithm 1 provide parallelism for calculating $\tilde{x}_i$'s and x_i^+'s. Let

$$x^k = \begin{bmatrix} x_1^k \\ \vdots \\ x_q^k \\ x_{q+1}^k \end{bmatrix} \tag{10}$$

denote the k^{th} iteration. Zhang *et al.* [2] suggested the following algorithm.

Algorithm 2 (Iteration k of the Corrected Implicit Method)

Step 1.
for $i = 1 : q$
$x_i^{k,0} = x_i^k$
for $j = 1 : j_i$
Solve $A_i(x^k)\Delta x_i^{k,j-1} = -f_i(x_i^{k,j-1}, x_{q+1}^k)$ for $\Delta x_i^{k,j-1}$
$x_i^{k,j} = x_i^{k,j-1} + \Delta x_i^{k,j-1}$
end
end
Step 2.
Calculate $S(x^k) = D(x^k) - \sum_{i=1}^q C_i(x^k)A_i^{-1}(x^k)B_i(x^k)$.
Solve $S(x^k)\Delta x_{q+1} = -f_{q+1}(x_1^{k,j_1}, \dots, x_q^{k,j_q}, x_{q+1}^k)$ for Δx_{q+1}.
$x_{q+1}^{k+1} = x_{q+1}^k + \Delta x_{q+1}$
Step 3.
for $i = 1 : q$
$x_i^{k+1} = x_i^{k,j_i} - A_i^{-1}(x^k)B_i(x^k)\Delta x_{q+1}$
end

The basic corrected implicit method is defined by $j_i = 1$ $(i = 1, \dots, q)$. The class of corrected implicit methods is a modification of the basic corrected implicit method such that it allows repetition of Step 1 "equationwise". The reason for this is the parallel bottleneck in Step 2 of Algorithm 1 or 2 [2]. Globalized versions of Algorithm 2 and their convergence analysis are given in [8].

3. THE BLOCK IMPLICIT LU ABS METHOD

The nonlinear ABS methods, a class of Brent-Brown type methods, were developed by Abaffy *et al.* [13], Abaffy and Galántai [14] (see also [15]). For the general nonlinear system

$$F(\mathbf{x}) = 0, \qquad \left(F = [f_1, \dots, f_n]^\top : R^n \to R^n\right), \tag{11}$$

the block ABS methods are defined in the following way.

Algorithm 3 (Iteration k of the nonlinear block ABS method)

$u^1 = x^k$, $H_1 = I_n$.
Choose $V = [V_1, \dots, V_r] \in R^{n\times n}(\det(V) \neq 0,\ V_j \in R^{n\times n_j},\ 1 \leq j \leq r(k))$.
for $i = 1 : r(k)$
$\eta_i = \sum_{j=1}^i \tau_{ji}u^j$ $(\tau_{ji} \geq 0,\ \sum_{j=1}^i \tau_{ji} = 1)$
$P_i = H_i^\top Z_i$ $(Z_i \in R^{n\times n_i}, \det(P_i^\top J(\eta_i)^\top V_i) \neq 0)$
$u^{i+1} = u^i - P_i(V_i^\top J(\eta_i)P_i)^{-1}V_i^\top F(u^i)$
$H_{i+1} = H_i - H_iJ(\eta_i)^\top V_i(W_i^\top H_iJ(\eta_i)^\top V_i)^{-1}W_i^\top H_i$ $(W_i \in R^{n\times n_i})$
end
$x^{k+1} = u^{r(k)+1}$.

Notice that the parameter matrices V,

$$W = [W_1, \dots, W_{r(k)}], \qquad Z = [Z_1, \dots, Z_{r(k)}],$$

and their partition may vary with k. The main features of the nonlinear ABS methods, similarly to other Brent-Brown methods [16], are the following. One major iteration solves a linear system "row" by "row". The "rows" of this linear system are built up using the last minor iteration u^i available. Each minor iteration u^i satisfies all previous equations.

Let the $n \times n$ unit matrix I_n be partitioned into r blocks as follows:

$$I_n = \left[E^{(1)}, \dots, E^{(r)}\right] \qquad \left(E^{(i)} \in R^{n \times n_i}\right). \tag{12}$$

The block implicit LU ABS method is then defined on the nonlinear system (11) as follows (see [14]).

Algorithm 4 (Iteration k of the nonlinear block implicit LU ABS method)

$u^1 = x^k$, $H_1 = I_n$
for $i = 1 : r$
  $P_i = H_i^\top E^{(i)}$
  $\eta_i = \sum_{j=1}^{i} \tau_{ji} u^j$ $(\tau_{ji} \geq 0, \sum_{j=1}^{i} \tau_{ji} = 1)$
  $u^{i+1} = u^i - P_i(E^{(i)T} J(\eta_i) P_i)^{-1} E^{(i)T} F(u^i)$
  $H_{i+1} = H_i - H_i J(\eta_i)^\top E^{(i)} (E^{(i)T} H_i J(\eta_i)^\top E^{(i)})^{-1} E^{(i)T} H_i$
end
$x^{k+1} = u^{r+1}$.

The block implicit LU method is a generalization of Brown's method [11] (for other block generalization of the Brent-Brown methods, see [17]).

Consider now one step of Algorithm 4 on the coupled nonlinear system

$$f(x,y) = 0, \qquad g(x,y) = 0, \tag{13}$$

where $x = [x_1^\top, \dots, x_q^\top]^\top$, $y = x_{q+1}$,

$$f(x,y) = \begin{bmatrix} f_1(x_1, x_{q+1}) \\ \vdots \\ f_q(x_q, x_{q+1}) \end{bmatrix} : R^n \to R^{n-n_{q+1}},$$

and

$$g(x,y) = f_{q+1}(x_1, \dots, x_{q+1}) : R^n \to R^{n_{q+1}}.$$

Notice that

$$f_x'(x,y) = \begin{bmatrix} A_1 & & & \\ & A_2 & & \\ & & \ddots & \\ & & & A_q \end{bmatrix}, \qquad f_y'(x,y) = \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_q \end{bmatrix}.$$

Let us partition u^i as follows:

$$u^i = \begin{bmatrix} u_1^i \\ u_2^i \end{bmatrix}, \qquad u^1 = \mathbf{x} = \begin{bmatrix} x \\ y \end{bmatrix}.$$

Then by direct calculation we have

$$u^2 = \begin{bmatrix} u_1^2 \\ u_2^2 \end{bmatrix} = \begin{bmatrix} x - [f_x'(x,y)]^{-1} f(x,y) \\ y \end{bmatrix},$$
$$S = g_y'(\eta_2) - g_x'(\eta_2)[f_x'(x,y)]^{-1} f_y'(x,y),$$

and

$$u^3 = \begin{bmatrix} u_1^2 + [f_x'(x,y)]^{-1} f_y'(x,y) S^{-1} g(u_1^2, y) \\ y - S^{-1} g(u_1^2, y) \end{bmatrix}.$$

Using the notations

$$u_1^2 = \begin{bmatrix} \tilde{x}_1 \\ \vdots \\ \tilde{x}_q \end{bmatrix}, \qquad u_2^3 = x_{q+1}^+, \qquad u_1^3 = \begin{bmatrix} x_1^+ \\ \vdots \\ x_q^+ \end{bmatrix},$$

and choosing $\eta_2 = \mathbf{x}$, we obtain Method 2 of Algorithm 1 (see [1]). In the notation of Algorithm 1, the block implicit LU ABS method takes the following form.

Algorithm 5

Step 1.
for $i = 1 : q$
Solve $A_i(x^k)\Delta x_i = -f_i(x_i^k, x_{q+1}^k)$ for Δx_i.
$x_i^{k,1} = x_i^k + \Delta x_i$
end
Step 2.
Calculate $S(x^k) = D(x^k) - \sum_{i=1}^q C_i(x^k)A_i^{-1}(x^k)B_i(x^k)$.
Solve $S(x^k)\Delta x_{q+1} = -f_{q+1}(x_1^{k,1}, \dots, x_q^{k,1}, x_{q+1}^k)$ for Δx_{q+1}.
$x_{q+1}^{k+1} = x_{q+1}^k + \Delta x_{q+1}$
Step 3.
for $i = 1 : q$
$x_i^{k+1} = x_i^{k,1} - A_i^{-1}(x^k)B_i(x^k)\Delta x_{q+1}$
end

This form is obviously identical with the basic corrected implicit method of Zhang *et al.* [2]. It is noted that a direct application of the block implicit LU ABS method to the system (1) also leads to Algorithm 5 due to the block diagonal structure of the block $q \times q$ principal submatrix of the Jacobian matrix (3).

THEOREM 1. *The block implicit method contains Method 2 of Algorithm 1 and Algorithm 2 for* $j_i = 1$ $(i = 1, \dots, q)$.

In addition to the convergence results mentioned earlier, we can also apply the local convergence analysis of Galántai [18]. We omit the details here.

All nonlinear block ABS methods terminate in $r + 1$ steps on linear systems of the form $F(x) = Ax - b = 0$ for arbitrary initial vector u^1. We now investigate linear systems of the form

$$Ax = \begin{bmatrix} A_1 & & & & B_1 \\ & A_2 & & & B_2 \\ & & \ddots & & \vdots \\ & & & A_q & B_q \\ C_1 & C_2 & \dots & C_q & D \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_q \\ x_{q+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_q \\ b_{q+1} \end{bmatrix}.$$

Algorithm 5 now has the form

Step 1.
for $i = 1 : q$
Solve $A_i\Delta u_i = -(A_i u_i^1 + B_i u_{q+1}^1 - b_i)$ for Δu_i.
$u_i^{1,1} = u_i^1 + \Delta u_i$
end
Step 2.
Calculate $S = D - \sum_{i=1}^q C_i A_i^{-1} B_i$.
Solve $S\Delta u_{q+1} = -(\sum_i^q C_i u_i^{1,1} + D u_{q+1}^1 - b_{q+1})$ for Δu_{q+1}.
$u_{q+1}^2 = u_{q+1}^1 + \Delta u_{q+1}$
Step 3.
for $i = 1 : q$
$u_i^2 = u_i^{1,1} - A_i^{-1}B_i\Delta u_{q+1}$
end

The domain decomposition method of Bjørstad and Widlund [3] for solving the Poisson problem

$$\begin{aligned} -\Delta u &= f(x,y), \qquad (x,y) \in \Omega, \\ u(x,y) &= g(x,y), \qquad (x,y) \in \partial\Omega, \end{aligned}$$

leads to a linear system of the form

$$\begin{bmatrix} A_{1,1} & 0 & 0 & & A_{1,q+1} \\ & A_{2,2} & 0 & & A_{2,q+1} \\ & & A_{3,3} & & A_{3,q+1} \\ & & & \ddots & \vdots \\ A_{1,q+1}^{\top} & A_{1,q+1}^{\top} & A_{2,q+1}^{\top} & \cdots & A_{q+1,q+1} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{q+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{q+1} \end{bmatrix}. \tag{14}$$

Assuming that u_{q+1} is known, the solution of the system reduces to the solution of subsystems

$$A_{i,i}u_i = b_i - A_{i,q+1}u_{q+1}, \qquad i = 1, \dots, q. \tag{15}$$

A reduced system of equations in u_q is obtained from equation (14) by eliminating the unknown vectors u_1 through u_q. Substitute

$$u_i = A_{i,i}^{-1}(b_i - A_{i,q+1}u_{q+1})$$

into block number $q+1$ of equation (14) to obtain the *capacitance system*

$$Cu_{q+1} = s_{q+1}, \tag{16}$$

with the *capacitance matrix*

$$C = A_{q+1,q+1} - \sum_{i=1}^{q} A_{i,q+1}^{\top} A_{i,i}^{-1} A_{i,q+1} \tag{17}$$

as coefficient matrix, and with right-hand side vector given by

$$s_{q+1} = b_{q+1} - \sum_{i=1}^{q} A_{i,q+1}^{\top} v_i, \tag{18}$$

where

$$A_{ii}v_i = b_i, \qquad i = 1, \dots, q. \tag{19}$$

The domain decomposition method consists of three steps in order: the solution of systems (19), the solution of the capacitance system (16), and finally, the solution of systems (15). The subsystems can be solved by any available Poisson solver.

It is easy to verify the following statement.

THEOREM 2. *The block implicit LU ABS method contains the capacitance matrix method of Bjørstad and Widlund, if* $u^1 = 0$, $A_{i,q+1} = B_i$, *and* $C_i = A_{i,q+1}^{\top}$.

4. COMPUTATIONAL RESULTS

The numerical experiments of Bertocchi and Spedicato [19] indicated that the block implicit LU ABS methods may be competitive on dense linear systems and vector machines. The experimental results of Zhang *et al.* [2] also showed that the corrected implicit methods, or equivalently the Hoyer-Schmidt or the implicit LU ABS method, are very effective on nonlinear systems of the form (1). Van de Velde [5] gives a very detailed implementation and performance analysis of the domain decomposition method of Bjørstad and Widlund on parallel computers, which also applies here.

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